ATP: structure, its role as an energy currency molecule. Types and significance of chemical bonds; Structure and properties of water; significance of pH and buffers

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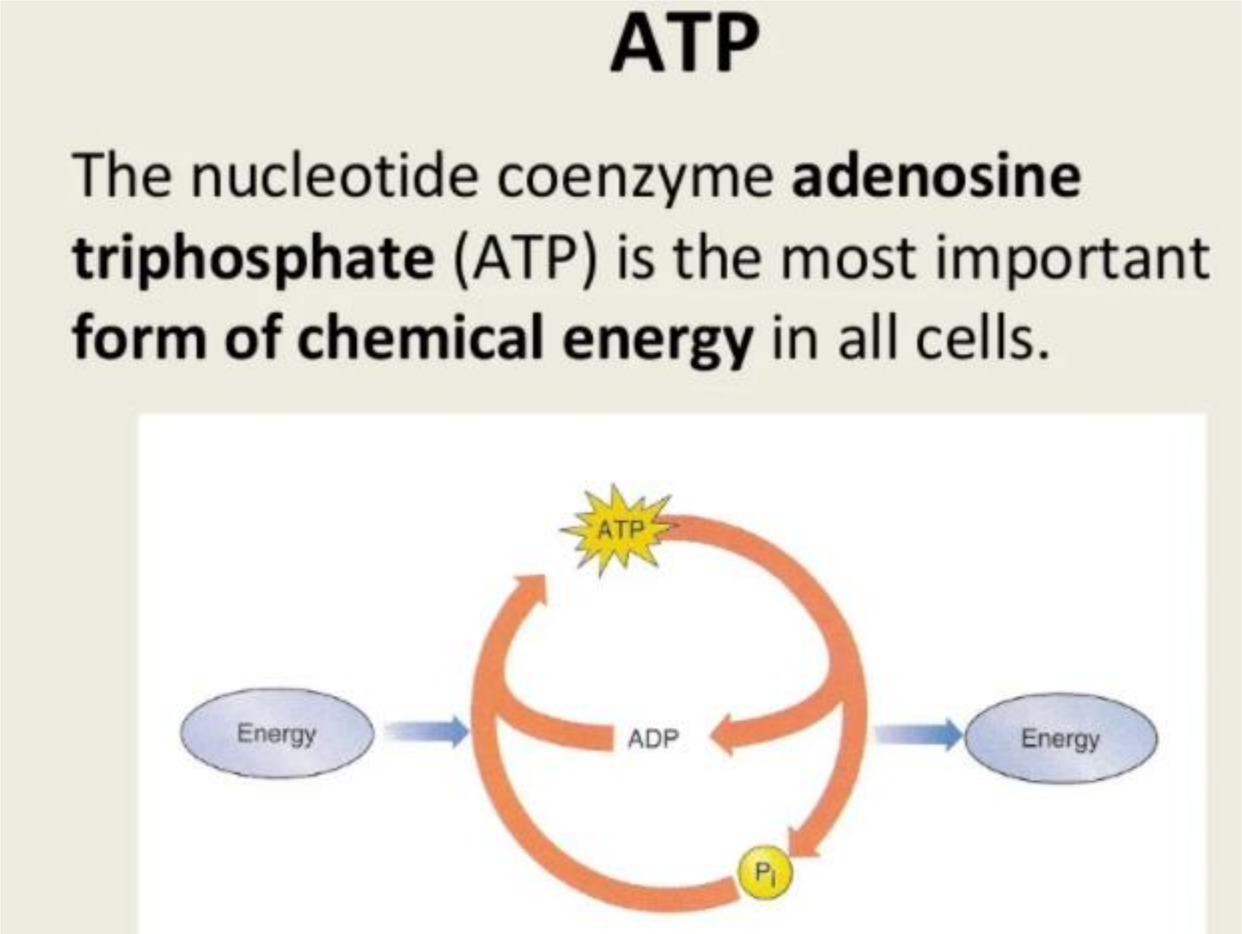
All living things including plants, animals, birds, insects, humans need energy for the proper functioning of cells, tissues and other organ systems. As we are aware that green plants, obtain their energy from the sunlight, and animals get their energy by feeding on these plants. Energy acts as a source of fuel. We, humans, gain energy from the food we eat, but how are the energy produced and stored in our body

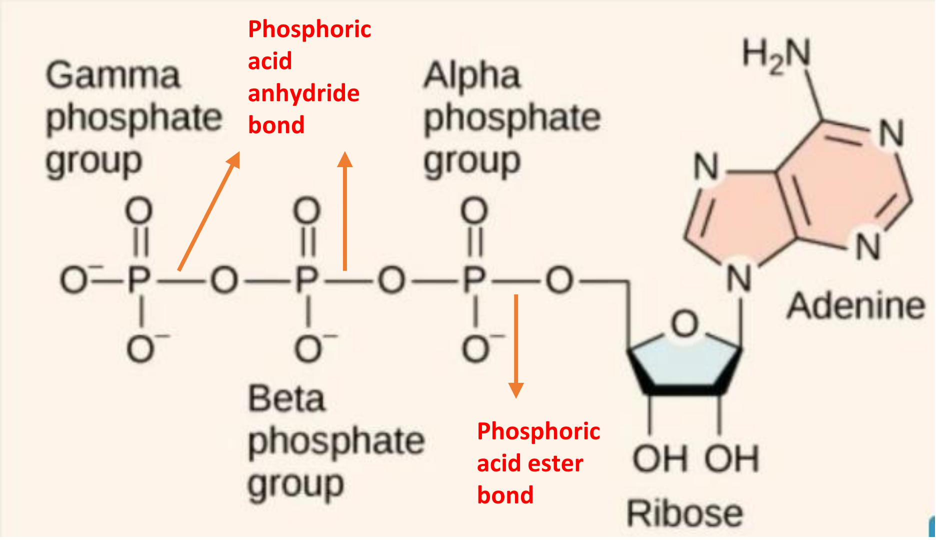


A living cell cannot store significant amounts of free energy. Excess free energy would result in an increase of heat in the cell, which would result in excessive thermal motion that could damage and then destroy the cell. Rather, a cell must be able to handle that energy in a way that enables the cell to store energy safely and release it for use only as needed. Living cells accomplish this by using the compound adenosine triphosphate (ATP). ATP is often called the “energy currency” of the cell, and, like currency, this versatile compound can be used to fill any energy need of the cell. How? It functions similarly to a rechargeable battery

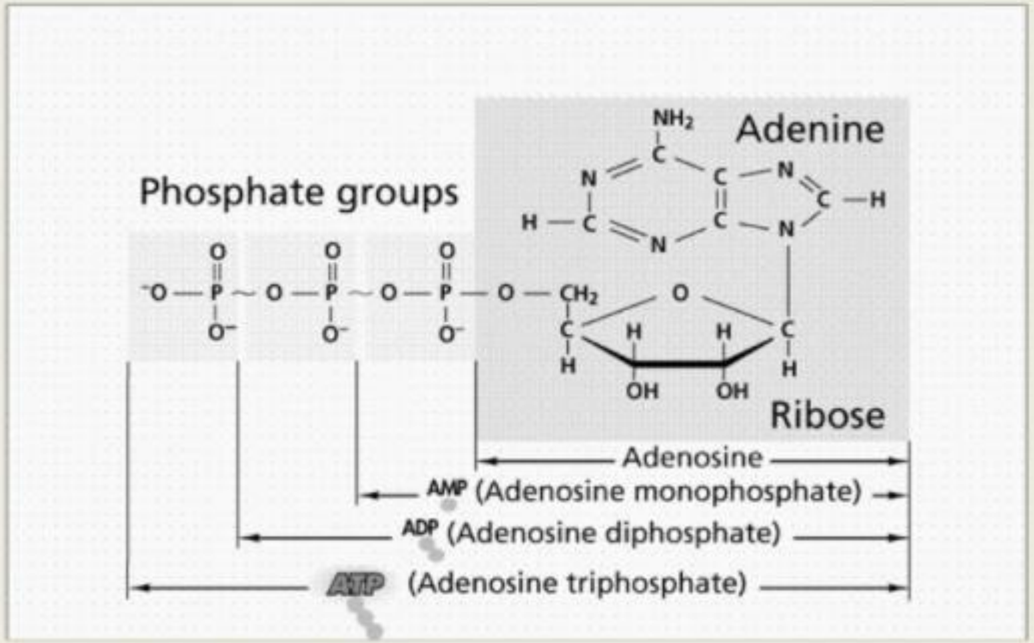
ATP molecules are largely composed of three essential components

- The pentose sugar molecule i.e. ribose sugar
- Nitrogen base- Adenine, attached to the first carbon of this sugar molecule
- The three phosphate groups which are attached in a chain to the 5th carbon of the pentose sugar. The phosphoryl groups, starting with the group closest to the ribose sugar, are referred to as the alpha, beta, and gamma phosphates. These phosphates play an important role in the activity of ATP

Phosphate residues in ATP Structure



ATP- Structure



ATP is a nucleoside triphosphate containing adenine, ribose, and three phosphate groups.

Mechanisms of ATP formation

There are two basic mechanism involved for ATP formation-

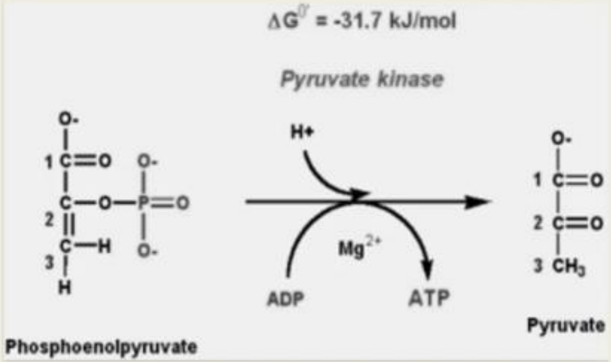
- Substrate level phosphorylation and
- Oxidative phosphorylation

1) Substrate level phosphorylation

- involves phosphorylation of ADP to form ATP at the expense of the energy of the parent substrate molecule without involving the electron transport chain.
- Substrate is a high energy compound as compared to the product, the surplus energy is used for ATP formation.

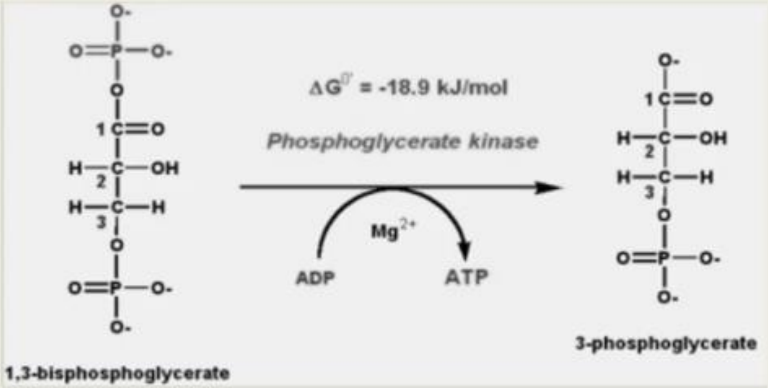
Substrate level phosphorylation in Glycolysis

- Conversion of phospho- enol -pyruvate to Pyruvate

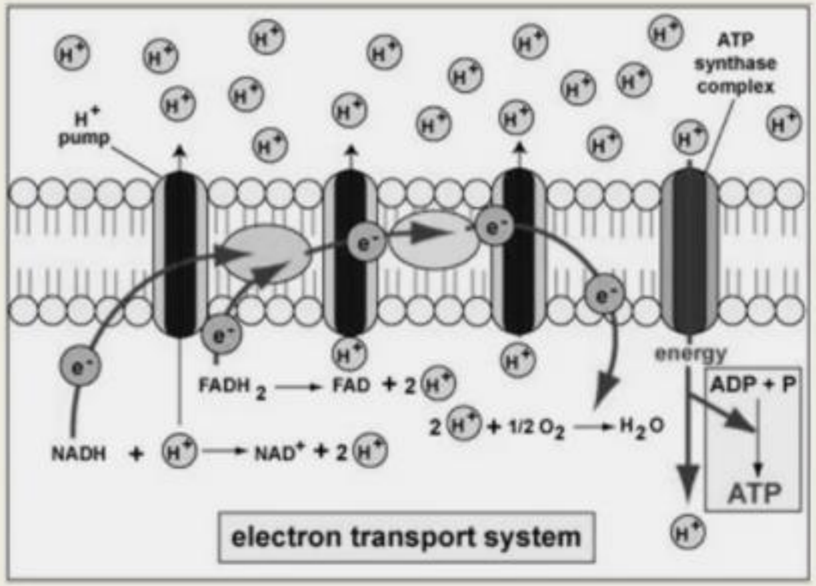


Substrate level phosphorylation in Glycolysis

- Conversion of 1,3 BPG to 3, Phosphoglycerate



2) ATP by Oxidative phosphorylation



- This process takes place in mitochondria and is energetically coupled to a proton gradient over a membrane.
- The H^+ gradients established by electron transport chain are used by the enzyme *ATP synthase* as a source of energy for direct linking of an inorganic phosphate to ADP.

Energy from ATP

- Hydrolysis is the process of breaking complex macromolecules apart
- The hydrolysis of ATP produces ADP, together with an inorganic phosphate ion (Pi), and the release of free energy
- To carry out life processes, ATP is continuously broken down into ADP, and like a rechargeable battery, ADP is continuously regenerated into ATP by the reattachment of a third phosphate group
- Obviously, energy must be infused into the system to regenerate ATP

Where does this energy come from?

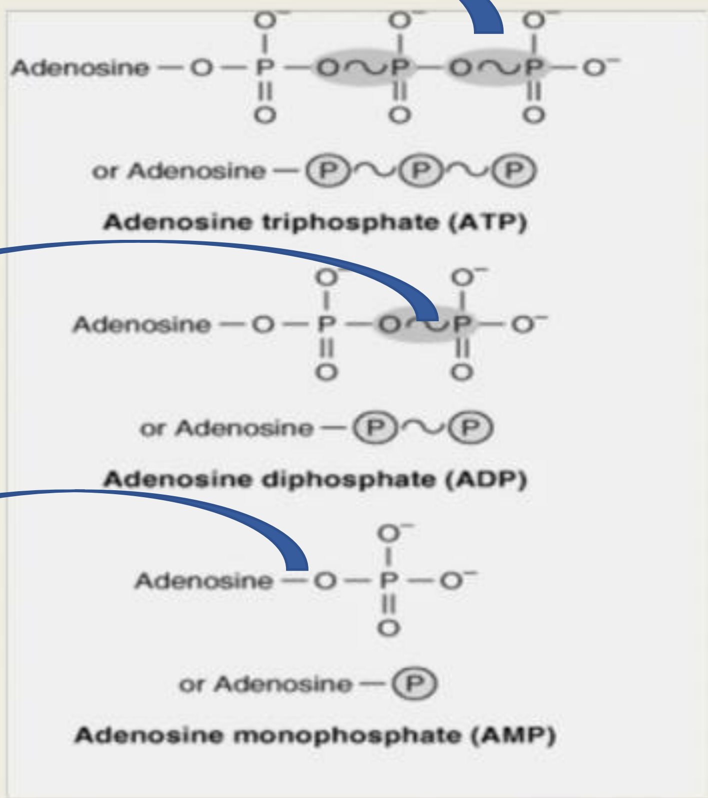
- In nearly every living thing on earth, the energy comes from the metabolism of glucose
- In this way, ATP is a direct link between the limited set of exergonic pathways of glucose catabolism and the multitude of endergonic pathways that power living cells
- How is Energy Produced by the ATP molecules? The three phosphate groups present in this ATP molecule are called high energy bonds as they are involved in the liberation of a huge amount of energy when they are broken
- This molecule provides energy for various life processes without which life cannot exist. It is used by various enzymes and structural proteins in cellular processes like biosynthetic reactions, cell divisions, etc
- This “energy currency of the cell” is produced during cellular respiration where a digested simple molecule of food is utilized

ATP Hydrolysis

-30KJ of energy releaded by breaking of anhydride bond

-30KJ of energy releaded by breaking of anhydride bond

-14KJ of energy released by breaking of ester bond



- ❑Adenosine attached to two or one phosphate residues is called **Adenosine di and mono phosphate** respectively.
- ❑The symbol ~ indicates that the group attached to the bond, on transfer to an appropriate acceptor, results in transfer of the larger quantity of free energy.
- ❑ For this reason, the term **group transfer potential** rather than "high-energy bond" is preferred .

Examples of coupling reactions

ATP can donate

- ❑single phosphate,
- ❑two phosphates or
- ❑even Adenosine moiety to suitable acceptors for the formation of important biological compounds.

A) Single phosphate transfer

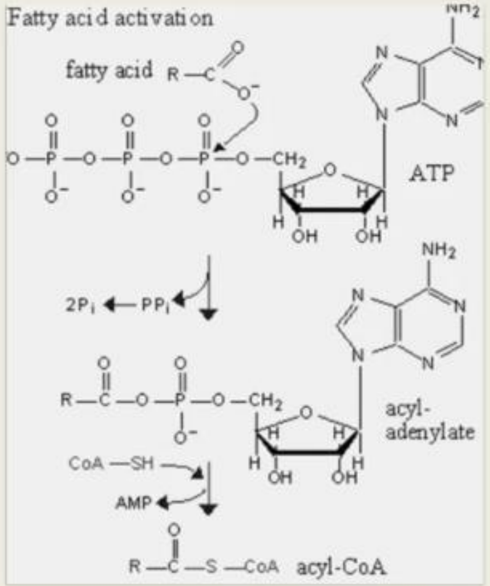
(1) Glucose + P_i → Glucose 6-phosphate + H_2O
($\Delta G^{0'} = +13.8$ kJ/mol)

(2) ATP → ADP + P_i ($\Delta G^{0'} = -30.5$ kJ/mol)

❑The phosphorylation of glucose to glucose 6-phosphate, the first reaction of Glycolysis, is highly endergonic and cannot proceed under physiologic conditions.
❑When (1) and (2) are coupled in a reaction catalyzed by hexokinase, phosphorylation of glucose readily proceeds in a highly exergonic reaction that under physiologic conditions is irreversible.

B) Transfer of two phosphate groups

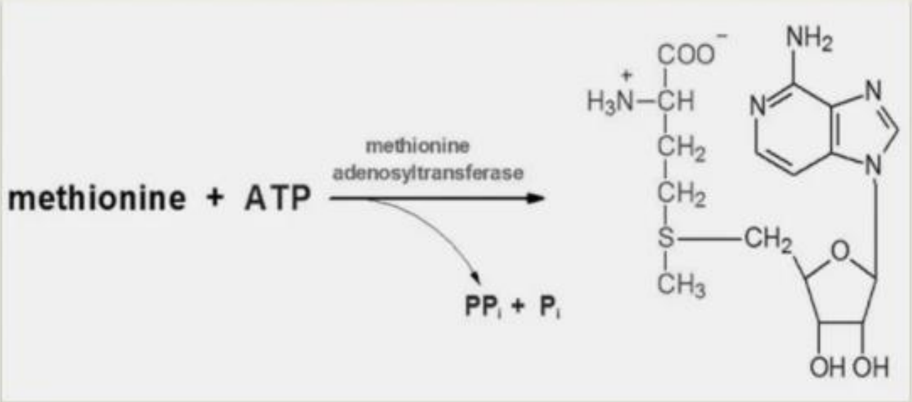
i) Activation of fatty acids



During the process of activation of fatty acid before oxidation, ATP is converted to AMP with the release of pyrophosphate, which can subsequently be hydrolyzed to inorganic phosphates.

C) Transfer of adenosine moiety

- This takes place during activation of Methionine to S-Adenosyl Methionine (Active Methionine), which is a methyl group donor in the body.



Importance of ATP Molecule in Metabolism

1. These ATP molecules can be recycled after every reaction
2. ATP molecule provides energy for both the exergonic and endergonic processes
3. ATP serves as an extracellular signalling molecule and acts as a neurotransmitter in both central and peripheral nervous systems
4. It is the only energy, which can be directly used for different metabolic process. Other forms of chemical energy need to be converted into ATP before they can be used
5. It plays an important role in the Metabolism – A life-sustaining chemical reactions including cellular division, fermentation, photosynthesis, photophosphorylation, aerobic respiration, protein synthesis, exocytosis, endocytosis and motility

Living things are made up of atoms, but in most cases, those atoms aren't just floating around individually. Instead, they're usually interacting with other atoms (or groups of atoms)

Why form chemical bonds? The basic answer is that atoms are trying to reach the most stable (lowest-energy) state that they can. Many atoms become stable when their valence shell is filled with electrons or when they satisfy the octet rule (by having eight valence electrons). If atoms don't have this arrangement, they'll "want" to reach it by gaining, losing, or sharing electrons via bonds

Ions and ionic bonds

Some atoms become more stable by gaining or losing an entire electron (or several electrons). When they do so, atoms form **ions**, or charged particles. Electron gain or loss can give an atom a filled outermost electron shell and make it energetically more stable

Forming ions

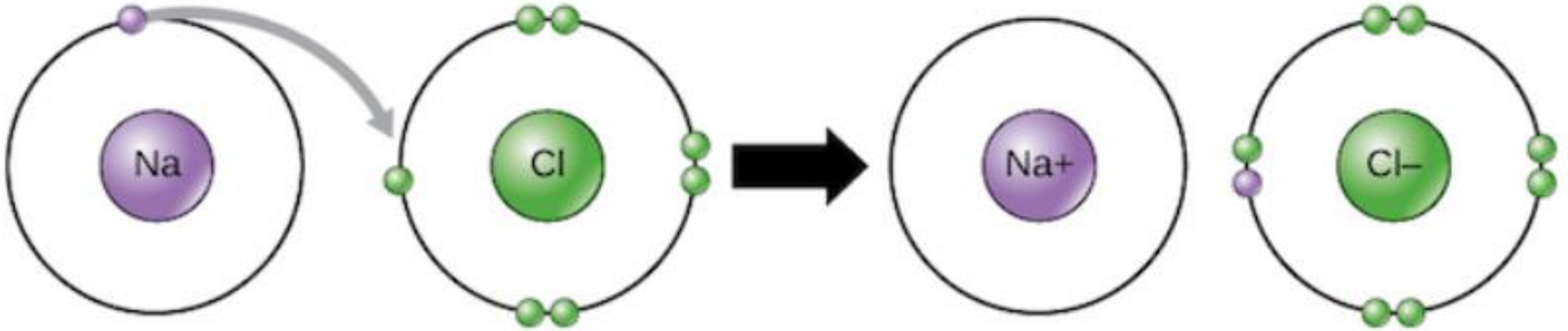
Ions come in two types. **Cations** are positive ions formed by losing electrons. For instance, a sodium atom loses an electron to become a sodium cation, Na^+

Negative ions are formed by electron gain and are called **anions**. Anions are named using the ending “-ide”: for example, the anion of chlorine Cl^- is called chloride.

When one atom loses an electron and another atom gains that electron, the process is called **electron transfer**. Sodium and chlorine atoms provide a good example of electron transfer.

Sodium (Na) only has one electron in its outer electron shell, so it is easier (more energetically favorable) for sodium to donate that one electron than to find seven more electrons to fill the outer shell. Because of this, sodium tends to lose its one electron, forming Na+start superscript, plus, end superscript.

Chlorine (Cl), on the other hand, has seven electrons in its outer shell. In this case, it is easier for chlorine to gain one electron than to lose seven, so it tends to take on an electron and become Cl^-



When sodium and chlorine are combined, sodium will donate its one electron to empty its shell, and chlorine will accept that electron to fill its shell. Both ions now satisfy the octet rule and have complete outermost shells. Because the number of electrons is no longer equal to the number of protons, each atom is now an ion and has a +1 (Na^+) or –1 (Cl^-) charge

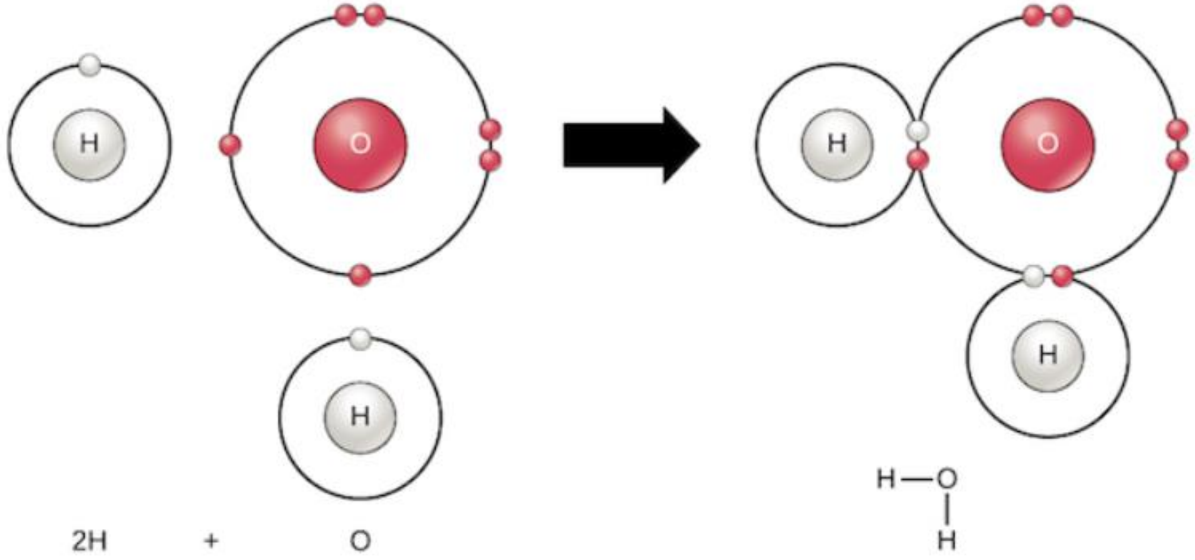
Covalent bonds

Another way atoms can become more stable is by sharing electrons (rather than fully gaining or losing them), thus forming **covalent bonds**. Covalent bonds are more common than ionic bonds in the molecules of living organisms.

For instance, covalent bonds are key to the structure of carbon-based organic molecules like our DNA and proteins. Covalent bonds are also found in smaller inorganic molecules, such as H2O, CO2, O2

One, two, or three pairs of electrons may be shared between atoms, resulting in single, double, or triple bonds, respectively. The more electrons that are shared between two atoms, the stronger their bond will be.

As an example of covalent bonding, let’s look at water. A single water molecule, H2O consists of two hydrogen atoms bonded to one oxygen atom. Each hydrogen shares an electron with oxygen, and oxygen shares one of its electrons with each



The shared electrons split their time between the valence shells of the hydrogen and oxygen atoms, giving each atom something resembling a complete valence shell (two electrons for H, eight for O). This makes a water molecule much more stable than its component atoms would have been on their own

Polar covalent bonds

There are two basic types of covalent bonds: polar and nonpolar. In a **polar covalent bond**, the electrons are unequally shared by the atoms and spend more time close to one atom than the other. Because of the unequal distribution of electrons between the atoms of different elements, slightly positive (δ+) and slightly negative (δ–) charges develop in different parts of the molecule.

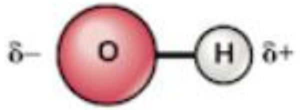
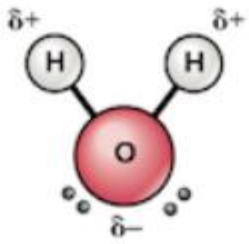
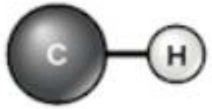
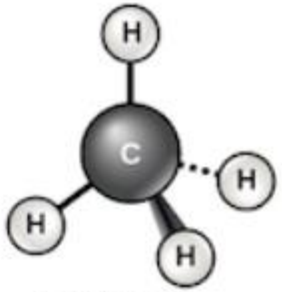
In a water molecule (above), the bond connecting the oxygen to each hydrogen is a polar bond. Oxygen is a much more **electronegative** atom than hydrogen, meaning that it attracts shared electrons more strongly, so the oxygen of water bears a partial negative charge (has high electron density), while the hydrogens bear partial positive charges (have low electron density)

Nonpolar covalent bonds

Nonpolar covalent bonds form between two atoms of the same element, or between atoms of different elements that share electrons more or less equally

example of a nonpolar covalent bond is found in methane CH4

Carbon has four electrons in its outermost shell and needs four more to achieve a stable octet. It gets these by sharing electrons with four hydrogen atoms, each of which provides a single electron. Reciprocally, the hydrogen atoms each need one additional electron to fill their outermost shell, which they receive in the form of shared electrons from carbon. Although carbon and hydrogen do not have exactly the same electronegativity, they are quite similar, so carbon-hydrogen bonds are considered nonpolar

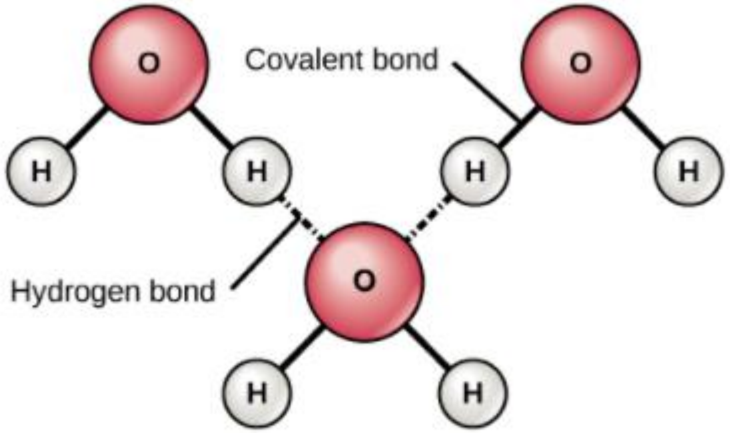
	Bond type	Molecular shape
Water	 Polar covalent	 Bent
Methane	 Nonpolar covalent	 Tetrahedral

HYDROGEN BONDS

Ionic and covalent bonds are strong bonds that require considerable energy to break. However, not all bonds between elements are ionic or covalent bonds. Weaker bonds can also form. These are attractions that occur between positive and negative charges that do not require much energy to break. Two weak bonds that occur frequently are hydrogen bonds and van der Waals interactions. These bonds give rise to the unique properties of water and the unique structures of DNA and proteins.

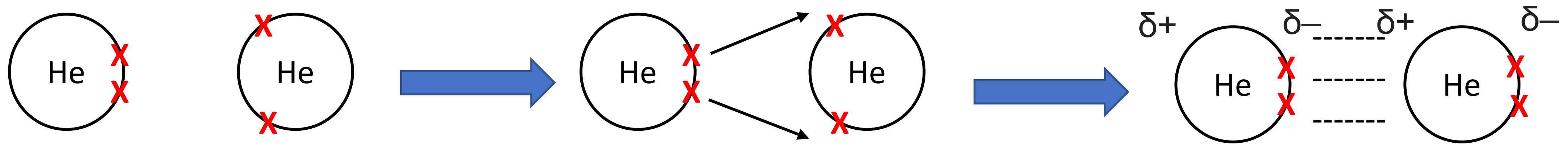
When polar covalent bonds containing a hydrogen atom form, the hydrogen atom in that bond has a slightly positive charge. This is because the shared electron is pulled more strongly toward the other element and away from the hydrogen nucleus. Because the hydrogen atom is slightly positive (δ+), it will be attracted to neighboring negative partial charges (δ–). When this happens, a weak interaction occurs between the δ+ charge of the hydrogen atom of one molecule and the δ– charge of the other molecule. This interaction is called a hydrogen bond. This type of bond is common; for example, the liquid nature of water is caused by the hydrogen bonds between water molecules (Figure 4). Hydrogen bonds give water the unique properties that sustain life. If it were not for hydrogen bonding, water would be a gas rather than a liquid at room temperature

Hydrogen bonds can form between different molecules and they do not always have to include a water molecule. Hydrogen atoms in polar bonds within any molecule can form bonds with other adjacent molecules. For example, hydrogen bonds hold together two long strands of DNA to give the DNA molecule its characteristic double-stranded structure. Hydrogen bonds are also responsible for some of the three-dimensional structure of proteins



VAN DER WAALS INTERACTIONS

Because electrons are in constant motion, there will be some moments when the electrons of an atom or molecule are clustered together, creating a partial negative charge in one part of the molecule (and a partial positive charge in another). If a molecule with this kind of charge imbalance is very close to another molecule, it can cause a similar charge redistribution in the second molecule, and the temporary positive and negative charges of the two molecules will attract each other



Push the electron to other side as
same charge repel

The Structure and Properties of Water

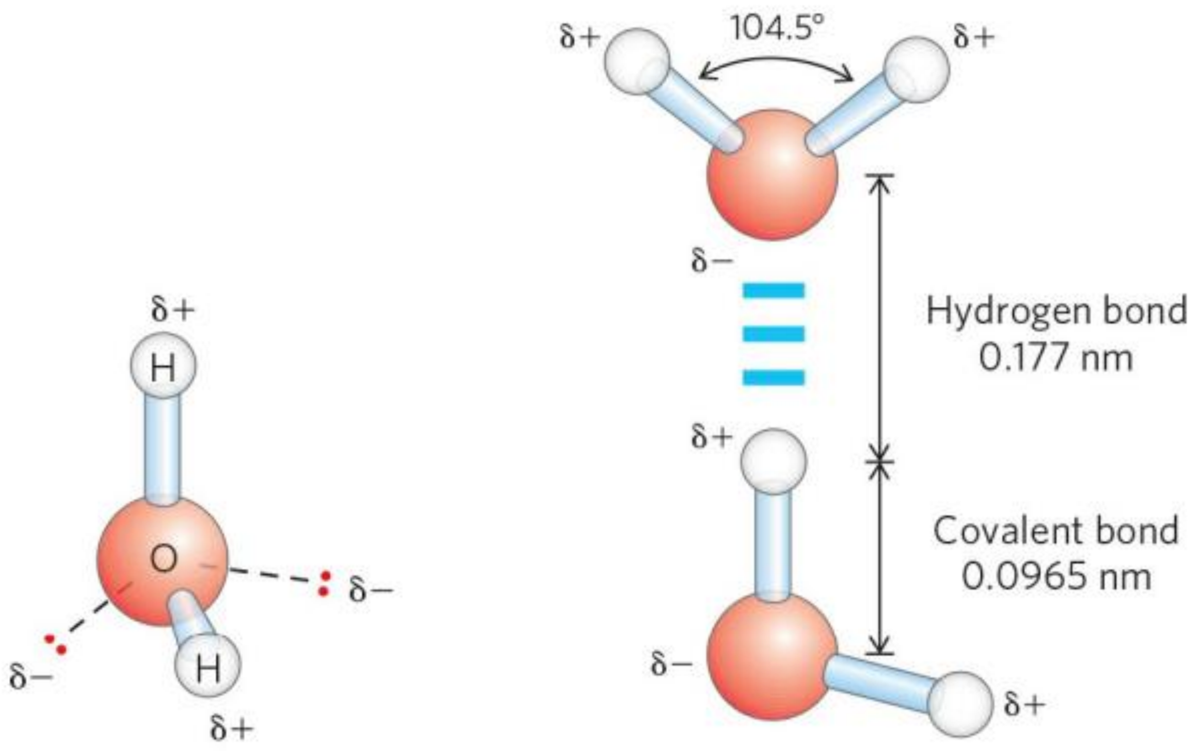
Key terms

Term	Meaning
Polar molecule	A neutral, or uncharged molecule that has an asymmetric internal distribution of charge, leading to partially positive and partially negative regions
Cohesion	The attraction of molecules for other molecules of the same kind
Adhesion	The attraction of molecules for other molecules of a different kind
Density	The mass per unit volume of a substance
Specific heat capacity	The amount of heat needed to raise the temperature of one gram of a substance by one degree Celsius
Heat of vaporization	The amount of energy needed to change one gram of a liquid substance to a gas at constant temperature

Selected physical properties of water

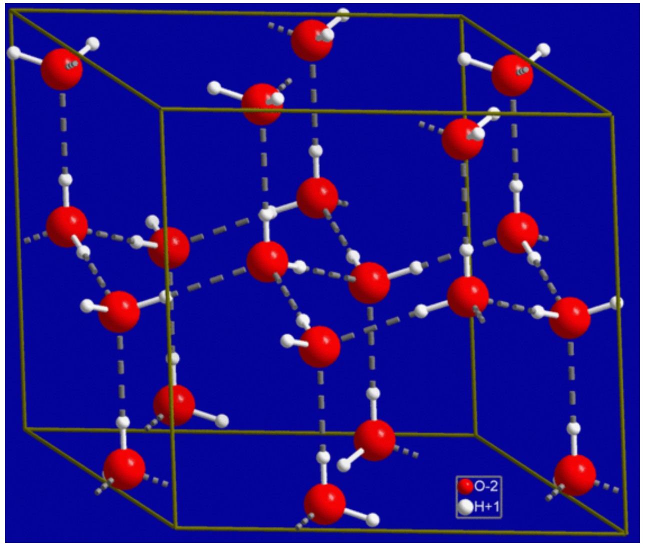
molar mass	18.0151 grams per mole
melting point	0.00 °C
boiling point	100.00 °C
maximum density (at 3.98 °C)	1.0000 grams per cubic centimetre
density (25 °C)	0.99701 grams per cubic centimetre
vapour pressure (25 °C)	23.75 torr
heat of fusion (0 °C)	6.010 kilojoules per mole
heat of vaporization (100 °C)	40.65 kilojoules per mole
heat of formation (25 °C)	−285.85 kilojoules per mole
entropy of vaporization (25 °C)	118.8 joules per °C mole
viscosity	0.8903 centipoise
surface tension (25 °C)	71.97 dynes per centimete

Refractive index (n_D)	1.3330
Viscosity	0.001 Pa s at 20 °C
Structure	
Crystal structure	Hexagonal
Molecular shape	Bent
Dipole moment	1.85 D


δ+
H
O
H
δ+
δ−
δ−
δ+
104.5°
δ+
δ+
δ−
Hydrogen bond
0.177 nm
δ+
Covalent bond
0.0965 nm
δ−
δ+

Solid Phase (Ice)

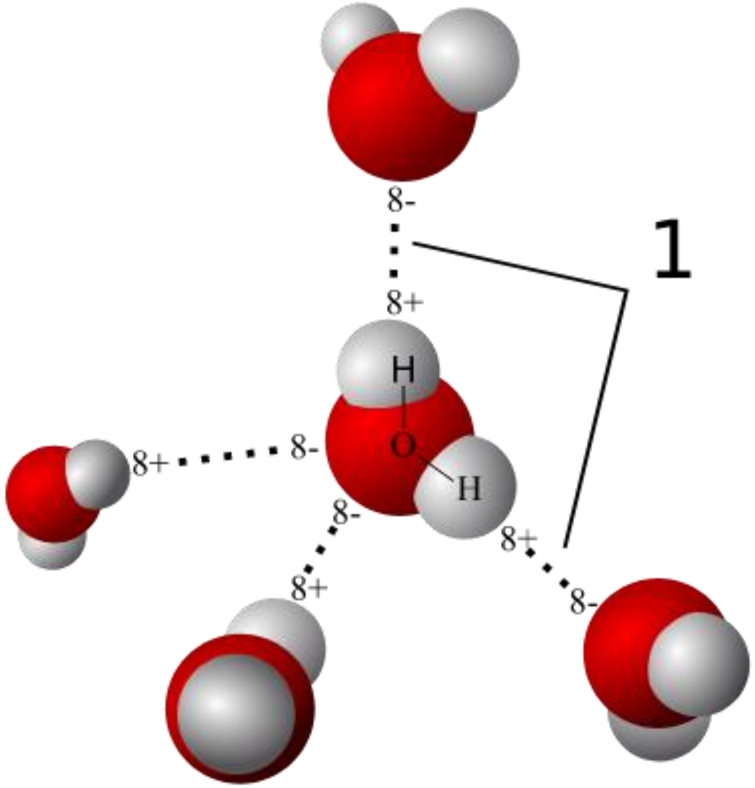
The solid phase of water is known as ice and commonly takes the structure of hard, amalgamated crystals, such as ice cubes, or of loosely accumulated granular crystals, such as snow. Unlike most other substances, water's solid form (ice) is *less* dense than its liquid form, as a result of the nature of its hexagonal packing within its crystalline structure. This lattice contains more space than when the molecules are in the liquid state



The hexagonal structure of ice As a naturally occurring crystalline inorganic solid with an ordered structure, ice is considered to be a mineral. It possesses a regular crystalline structure based on the molecular structure of water, which consists of a single oxygen atom covalently bonded to two hydrogen atoms: H-O-H

Liquid Phase (Water)

Water is primarily a liquid under standard conditions (25 degrees Celsius and 1 atm of pressure). This characteristic could not be predicted by its relationship to other, gaseous hydrides of the oxygen family in the periodic table, such as hydrogen sulfide. The elements surrounding oxygen in the periodic table – nitrogen, fluorine, phosphorus, sulfur, and chlorine – all combine with hydrogen to produce gases under standard conditions. Water forms a liquid instead of a gas because oxygen is more electronegative than the surrounding elements, with the exception of fluorine. Oxygen attracts electrons much more strongly than does hydrogen, resulting in a partial positive charge on the hydrogen atoms and a partial negative charge on the oxygen atom. The presence of such a charge on each of these atoms gives a water molecule a net dipole moment



Gas Phase (Water Vapor)

The gaseous phase of water is known as water vapor (or steam) and is characterized by a transparent cloud. Water also exists in a rare fourth state called supercritical fluid, which occurs only in extremely uninhabitable conditions. When water achieves a specific critical temperature and a specific critical pressure (647 K and 22.064 MPa), the liquid and gas phases merge into one homogeneous fluid phase that shares properties of both gas and liquid

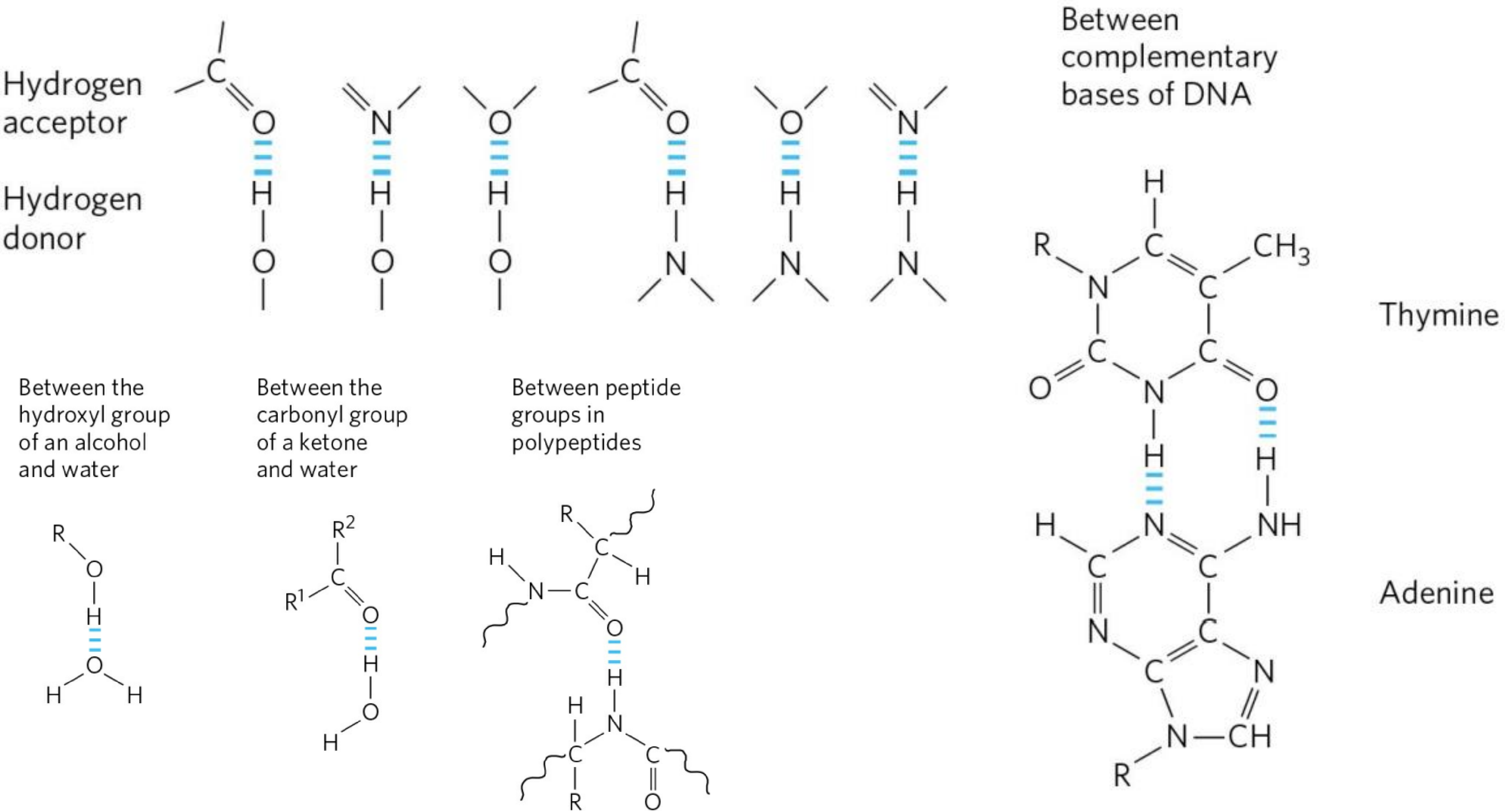
1. **Water is polar.** Water molecules are polar, with partial positive charges on the hydrogens, a partial negative charge on the oxygen, and a bent overall structure. This is because oxygen is more *electronegative*, meaning that it is better than hydrogen at attracting electrons.
2. **Water is an excellent solvent.** Water has the unique ability to dissolve many polar and ionic substances. This is important to all living things because, as water travels through the water cycle, it takes many valuable nutrients along with it!
3. **Water has high heat capacity.** It takes a lot of energy to raise the temperature of a certain amount of water by a degree, so water helps with regulating temperature in the environment. For example, this property allows the temperature of water in a pond to stay relatively constant from day to night, regardless of the changing atmospheric temperature.
4. **Water has high heat of vaporization.** Humans (and other animals that sweat) use water's high heat of vaporization to cool off. Water is converted from its liquid form to steam when the heat of vaporization is reached. Since sweat is made mostly of water, the evaporating water absorbs excess body heat, which is released into the atmosphere. This is known as *evaporative cooling*
5. **Water has cohesive and adhesive properties.** Water molecules have strong *cohesive* forces due to their ability to form hydrogen bonds with one another. Cohesive forces are responsible for *surface tension*, the tendency of a liquid's surface to resist rupture when placed under tension or stress. Water also has *adhesive* properties that allow it to stick to substances other than itself.

These cohesive and adhesive properties are essential for fluid transport in many forms of life. For example, they allow nutrients to be transported to the top of a tree against the force of gravity.

6. **Water is less dense as a solid than as a liquid.** As water freezes, the molecules form a crystalline structure that spaces the molecules further apart than in liquid water. This means that ice is less dense than liquid water, which is why it floats

This property is important, as it keeps ponds, lakes, and oceans from freezing solid and allows life to continue to thrive under the

Water Forms Hydrogen Bonds with Polar Solute



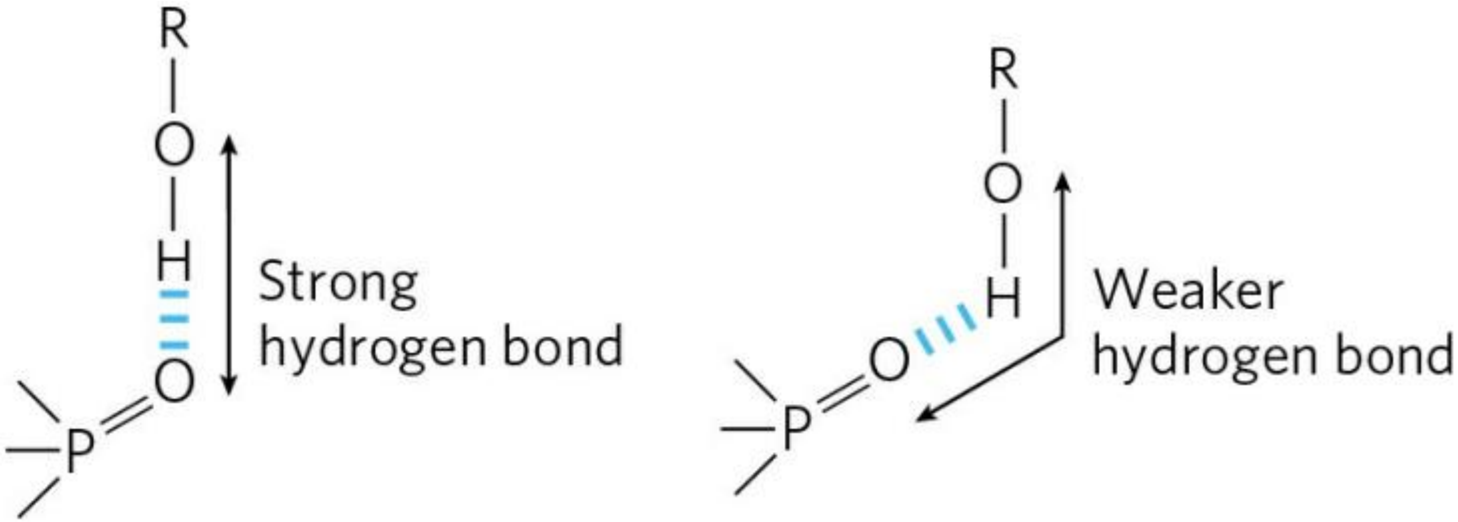
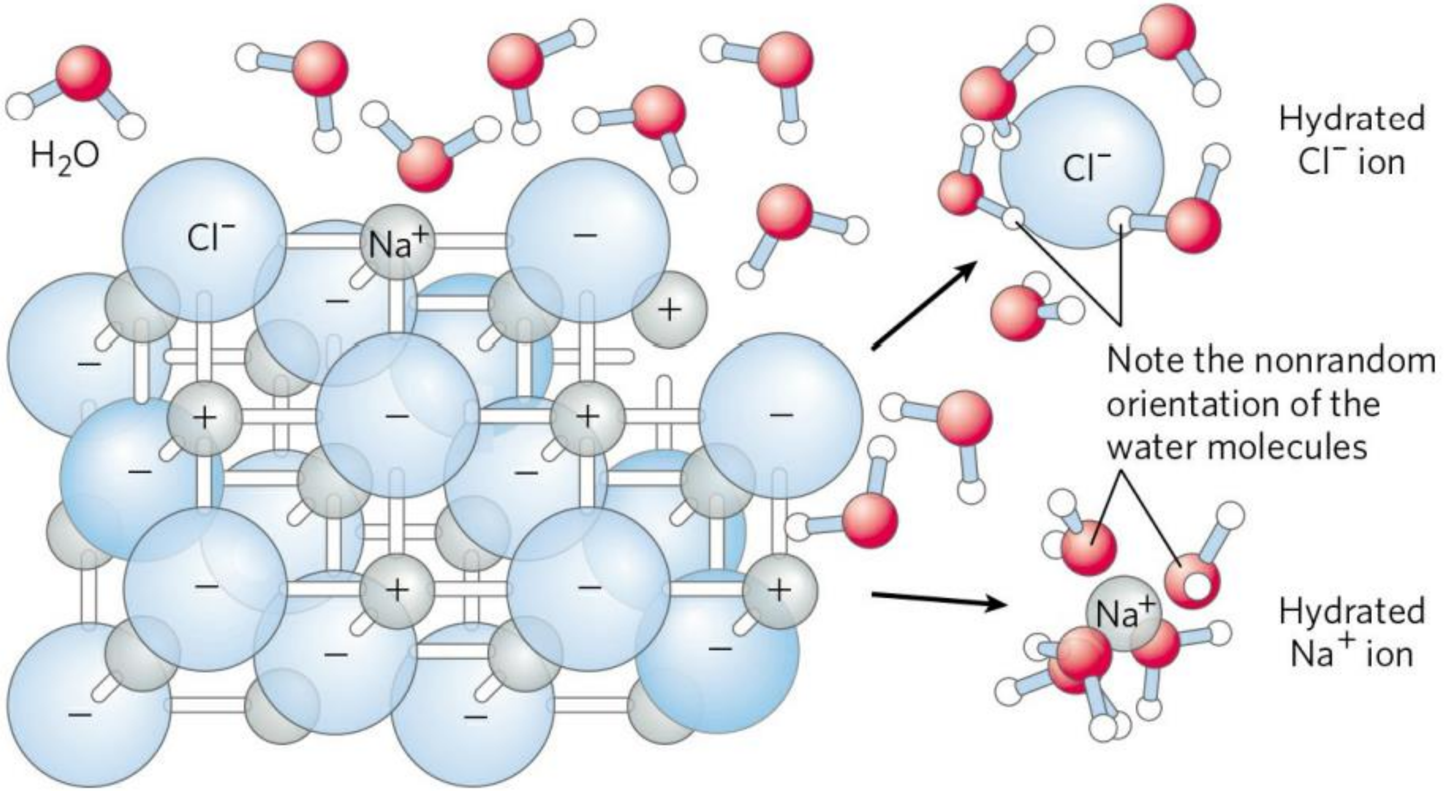


FIGURE 2-5 Directionality of the hydrogen bond. The attraction between the partial electric charges (see Fig. 2-1) is greatest when the three atoms involved in the bond (in this case O, H, and O) lie in a straight line. When the hydrogen-bonded moieties are structurally constrained (when they are parts of a single protein molecule, for example), this ideal geometry may not be possible and the resulting hydrogen bond is weaker.

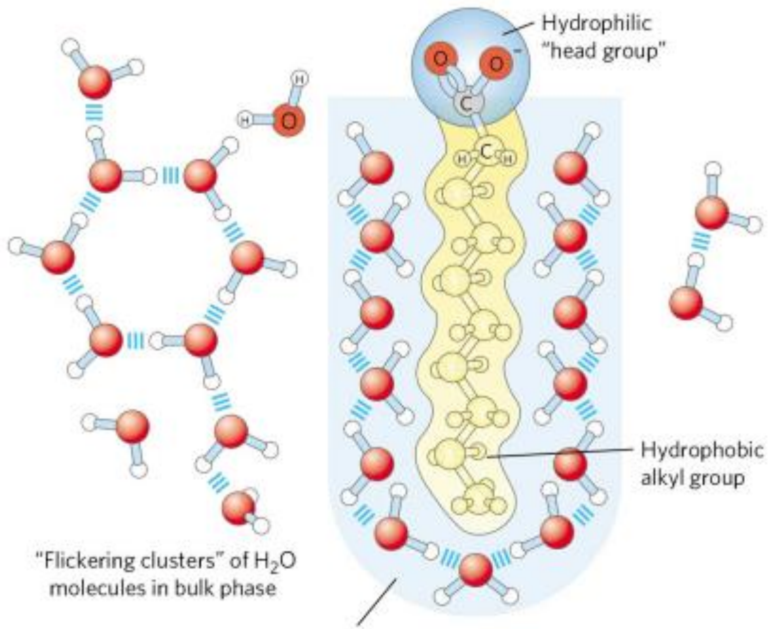
Water Interacts Electrostatically with Charged Solutes

Water is a polar solvent. It readily dissolves most biomolecules, which are generally charged or polar compounds (Table 2-2); compounds that dissolve easily in water are hydrophilic (Greek, "water-loving"). In contrast, nonpolar solvents such as chloroform and benzene are poor solvents for polar biomolecules but easily dissolve those that are hydrophobic—nonpolar molecules such as lipids and waxes. Water dissolves salts such as NaCl by hydrating and stabilizing the Na + and Cl − ions, weakening the electrostatic interactions between them and thus counteracting their tendency to associate in a crystalline lattice (Fig. 2-6). Water also readily dissolves charged biomolecules, including compounds with functional groups such as ionized carboxylic acids (—COO−), protonated amines , and phosphate esters or anhydrides. Water replaces the solute-solute hydrogen bonds linking these biomolecules to each other with solute-water hydrogen bonds, thus screening the electrostatic interactions between solute molecules

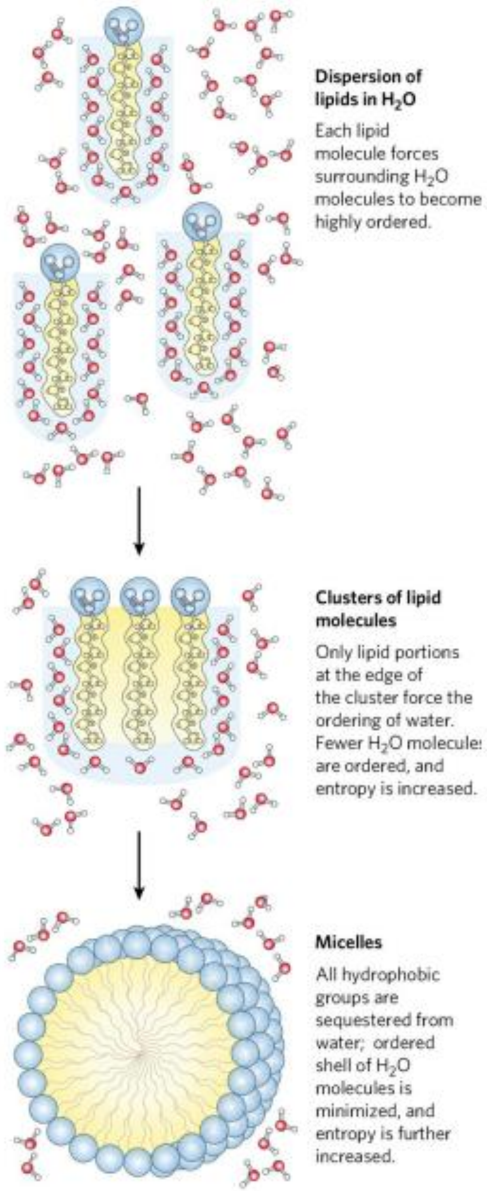


Nonpolar Compounds Force Energetically Unfavorable Changes in the Structure of Water

Amphipathic compounds contain regions that are polar (or charged) and regions that are nonpolar (Table 2-2). When an amphipathic compound is mixed with water, the polar, hydrophilic region interacts favorably with the water and tends to dissolve, but the nonpolar, hydrophobic region tends to avoid contact with the water (Fig. 2-7a). The nonpolar regions of the molecules cluster together to present the smallest hydrophobic area to the aqueous solvent, and the polar regions are arranged to maximize their interaction with the solvent (Fig. 2-7b), a phenomenon called the hydrophobic effect. These stable structures of amphipathic compounds in water, called micelles, may contain hundreds or thousands of molecules. The forces that hold the nonpolar regions of the molecules together are sometimes referred to as hydrophobic interactions, although this terminology can be confusing because the strength of the interactions is not due to any intrinsic attraction between nonpolar moieties. Rather, it results from the system's achieving the greatest thermodynamic stability by minimizing the number of ordered water molecules required to surround hydrophobic portions of the solute molecules



(a)



ACIDS, BASES AND SALTS

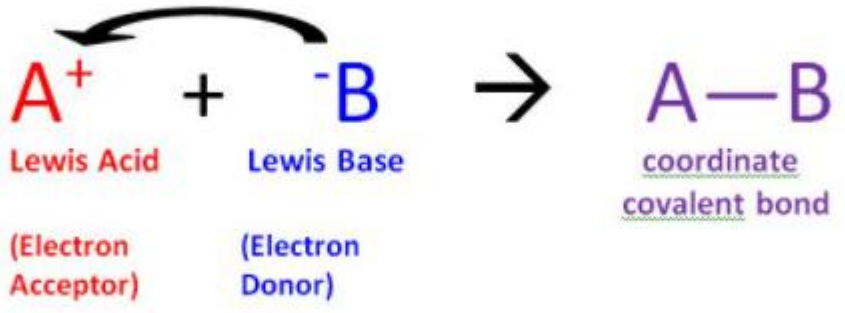
An acid is a substance which furnishes hydrogen ions (H^+) when dissolved in water. For example, in its aqueous solution hydrochloric HCl (aq) dissociates as: $HCl(aq) \longrightarrow H^+(aq) + Cl^-(aq)$

Some examples of acids are:
(i) Hydrochloric acid (HCl) in gastric juice
(ii) Carbonic acid (H_2CO_3) in soft drinks
(iii) Ascorbic acid (vitamin C) in lemon and many fruits

Bases

A base is a substance which furnishes hydroxide ions (OH^-) when dissolved in water. For example, sodium hydroxide NaOH (aq), in its aqueous solutions, dissociates as: $NaOH(aq) \longrightarrow Na^+(aq) + OH^-(aq)$
The term 'alkali' is often used for water soluble bases
Some examples of bases are
(i) Sodium hydroxide (NaOH) or caustic soda used in washing soaps
(ii) Potassium hydroxide (KOH) or potash used in bathing soaps
(iii) Calcium hydroxide ($Ca(OH)_2$) or lime water used in white wash
(iv) Magnesium hydroxide ($Mg(OH)_2$) or milk of magnesia used to control acidity
(v) Ammonium hydroxide (NH_4OH) used in hair dyes

•Lewis Acid: a species that accepts an electron pair (i.e., an electrophile) and will have vacant orbitals
•Lewis Base: a species that donates an electron pair (i.e., a nucleophile) and will have lone-pair electrons



•Various species can act as Lewis acids. All cations are Lewis acids since they are able to accept electrons. (e.g., Cu^{2+}, Fe^{2+}, Fe^{3+})
•An atom, ion, or molecule with an incomplete octet of electrons can act as an Lewis acid (e.g., BF_3, AlF_3)

Lewis Bases donate an electron pair. Lewis Bases are Nucleophilic meaning that they "attack" a positive charge with their lone pair
An atom, ion, or molecule with a lone-pair of electrons can thus be a Lewis base. Each of the following anions can "give up" their electrons to an acid, e.g., OH−OH−, CN−CN−, CH3COO−CH3COO−, :NH3:NH3, H2O:H2O:, CO:

Amphoterism

As of now you should know that acids and bases are distinguished as two separate things however some substances can be both an acid and a base. You may have noticed this with water, which can act as both an acid or a base. This ability of water to do this makes it an amphoteric molecule. Water can act as an acid by donating its proton to the base and thus becoming its conjugate acid, OH-. However, water can also act as a base by accepting a proton from an acid to become its conjugate base, H_3O^+.

- Water acting as an Acid:

$$H_2O + NH_3 \rightarrow NH_4^+ + OH^-$$

- Water acting as a Base:

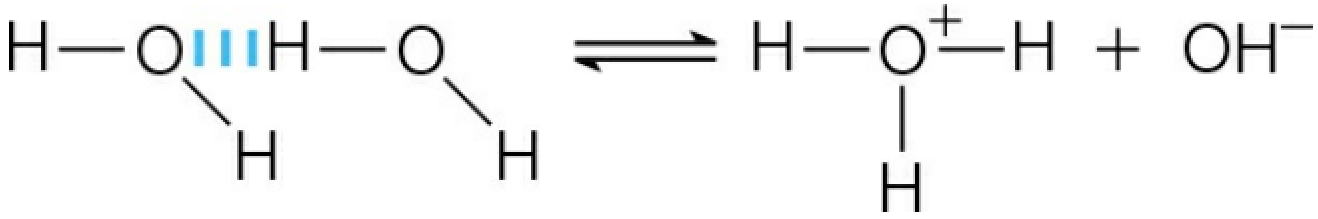
$$H_2O + HCl \rightarrow Cl^- + H_3O^+$$

pH, quantitative measure of the acidity or basicity of aqueous or other liquid solutions. The term, widely used in chemistry, biology, and agronomy, translates the values of the concentration of the hydrogen ion—which ordinarily ranges between about 1 and 10^{-14} gram-equivalents per litre—into numbers between 0 and 14. In pure water, which is neutral (neither acidic nor alkaline), the concentration of the hydrogen ion is 10^{-7} gram-equivalents per litre, which corresponds to a pH of 7. A solution with a pH less than 7 is considered acidic; a solution with a pH greater than 7 is considered basic, or alkalin

The measurement was originally used by the Danish biochemist S.P.L. Sørensen to represent the hydrogen ion concentration, expressed in equivalents per litre, of an aqueous solution: pH = $-\log[H^+]$ (in expressions of this kind, enclosure of a chemical symbol within square brackets denotes that the concentration of the symbolized species is the quantity being considered)

Pure Water Is Slightly Ionized Water molecules have a slight tendency to undergo reversible ionization to yield a hydrogen ion (a proton) and a hydroxide ion, giving the equilibrium Although we commonly show the dissociation product of water as H+ , free protons do not exist in solution; hydrogen ions formed in water are immediately hydrated to form hydronium ions (H3O+). Hydrogen bonding between water molecules makes the hydration of dissociating protons virtually instantaneous

$$H_2O \rightleftharpoons H^+ + OH^-$$



The Ionization of Water Is Expressed by an Equilibrium Constant

The position of equilibrium of any chemical reaction is given by its equilibrium constant, Keq (sometimes expressed simply as K). For the generalized reaction the equilibrium constant Keq can be defined in terms of the concentrations of reactants (A and B) and products (C and D) at equilibrium

$$A + B \rightleftharpoons C + D$$

$$K_{eq} = \frac{[C]_{eq}\,[D]_{eq}}{[A]_{eq}\,[B]_{eq}}$$

$$H_2O \rightleftharpoons H^+ + OH^-$$

$$K_{eq} = \frac{[H^+][OH^-]}{[H_2O]}$$

In pure water at 25 °C, the concentration of water is 55.5 M—grams of H2O in 1 Ldivided by its gram molecular weight: (1,000 g/L)/(18.015 g/mol)—and is essentially constant in relation to the very low concentrations of H+ and OH− , namely 1 × 10 −7 M. Accordingly, we can substitute 55.5 M in the equilibrium constant expression (Eqn 2-3) to yield

$$K_{eq} = \frac{[H^+][OH^-]}{[55.5\,M]}$$

$$(55.5\,M)\ (K_{eq}) = [H^+][OH^-] = K_w$$

where Kw designates the product (55.5 M)(Keq), the ion product of water at 25 °C. The value for Keq , determined by electrical-conductivity measurements of pure water, is 1.8 × 10 −16 M at 25 °C. Substituting this value for Keq in Equation 2-4 gives the value of the ion product of water

$$\begin{aligned} K_w &= [H^+]\ [OH^-] = (55.5\,M)\ (1.8 \times 10^{-16}\,M) \\ &= 1.0 \times 10^{-14}\,M^2 \end{aligned}$$

Thus the product [H+][OH−] in aqueous solutions at 25 °C always equals 1×10^{-14} M^2 . When there are exactly equal concentrations of H+ and OH− , as in pure water, the solution is said to be at neutral pH. At this pH, the concentrations of H+ and OH− can be calculated from the ion product of water as follows

$$K_w = [H^+][OH^-] = [H^+]^2 = [OH^-]^2$$

$$[H^+] = \sqrt{K_w} = \sqrt{1 \times 10^{-14} M^2}$$

$$[H^+] = [OH^-] = 10^{-7}\,M$$

As the ion product of water is constant, whenever [H+] is greater than 1×10^{-7} M, [OH–] must be less than 1×10^{-7} M, and vice versa. When [H+] is very high, as in a solution of hydrochloric acid, [OH–] must be very low. From the ion product of water we can calculate [H+] if we know [OH–], and vice versa

WORKED EXAMPLE 2-3 Calculation of $[H^+]$

What is the concentration of H^+ in a solution of 0.1 M NaOH?

Solution: We begin with the equation for the ion product of water:

$$K_w = [H^+][OH^-]$$

With $[OH^-] = 0.1$ M, solving for $[H^+]$ gives

$$[H^+] = \frac{K_w}{[OH^-]} = \frac{1\times10^{-14}\,M^2}{0.1\,M} = \frac{10^{-14}\,M^2}{10^{-1}\,M} = 10^{-13}\,M$$

WORKED EXAMPLE 2-4 Calculation of $[OH^-]$

What is the concentration of OH^- in a solution with an H^+ concentration of 1.3×10^{-4} M?

Solution: We begin with the equation for the ion product of water:

$$K_w = [H^+][OH]^-$$

With $[H^+] = 1.3 \times 10^{-4}$ M, solving for $[OH^-]$ gives

$$[OH^-] = \frac{K_w}{[H^+]} = \frac{1\times10^{-14}\,M^2}{0.00013\,M} = \frac{10^{-14}\,M^2}{1.3\times10^{-4}\,M} = 7.7\times10^{-11}\,M$$

The pH Scale Designates the H+ and OH− Concentrations The ion product of water, Kw, is the basis for the pH scale (Table 2-6). It is a convenient means of designating the concentration of H+ (and thus of OH−) in any aqueous solution in the range between 1.0 M H+ and 1.0 M OH− . The term pH is defined by the expression

$$pH = \log \frac{1}{[H^+]} = -\log\ [H^+]$$

TABLE 2-6 The pH Scale

$[H^+]$ (M)	pH	$[OH^-]$ (M)	pOH[a]
10^0 (1)	0	10^{-14}	14
10^{-1}	1	10^{-13}	13
10^{-3}	2	10^{-11}	11
10^{-}	4	10^{-10}	10
10^{-5}	5	10^{-9}	9
10^{-6}	6	10^{-8}	8
10^{-7}	7	10^{-7}	7
10^{-8}	8	10^{-6}	6
10^{-9}	9	10^{-5}	5
10^{-10}	10	10^{-4}	4
10^{-11}	11	10^{-3}	3
10^{-12}	12	10^{-2}	2
10^{-13}	13	10^{-1}	1
10^{-14}	14	10^0 (1)	0